

exact/norm bonds: 12-13 13-14 13-15 13-16 14-17 15-24 16-31 17-18 18-19 19-20 20-21 21-22 22-23 24-25 25-26 26-27 27-28 28-29 29-30 31-32 32-33 33-34 34-35 35-36 36-37

 Match level:
 1:Atom
 2:Atom
 3:Atom
 4:Atom
 5:Atom
 6:Atom
 7:Atom
 8:Atom
 9:Atom
 10:CLASS

 11:CLASS
 12:CLASS
 13:CLASS
 15:CLASS
 15:CLASS
 17:CLASS
 18:CLASS

 19:CLASS
 20:CLASS
 21:CLASS
 23:CLASS
 24:CLASS
 25:CLASS
 26:CLASS

 27:CLASS
 28:CLASS
 29:CLASS
 30:CLASS
 31:CLASS
 32:CLASS
 33:CLASS
 34:CLASS

 35:CLASS
 36:CLASS
 37:CLASS
 31:CLASS
 32:CLASS
 33:CLASS
 34:CLASS

4 ANSWERS

L1 STRUCTURE UPLOADED

=> s 11 sss full FULL SEARCH INITIATED 11:19:43 FILE 'REGISTRY' FULL SCREEN SEARCH COMPLETED - 772 TO ITERATE

100.0% PROCESSED 772 ITERATIONS SEARCH TIME: 00.00.01

L2 =>

ring nodes :

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1 2 3 4 5 6 7 8 9 13 14 15 16 17

4 SEA SSS FUL L1

```
ring/chain nodes: 10 \quad 11 \quad 12 \\ \text{ring/chain bonds}: \\ 7-11 \quad 8-12 \quad 9-10 \quad 12-13 \\ \text{ring bonds}: \\ 1-2 \quad 1-6 \quad 2-3 \quad 3-4 \quad 4-5 \quad 4-7 \quad 5-6 \quad 5-9 \quad 7-8 \quad 8-9 \quad 13-14 \quad 13-17 \quad 14-15 \quad 15-16 \quad 16-17 \\ \text{exact bonds}: \\ 4-7 \quad 5-9 \quad 7-8 \quad 7-11 \quad 8-9 \quad 8-12 \quad 9-10 \quad 12-13 \\ \text{normalized bonds}: \\ \end{array}
```

 $1-2 \quad 1-6 \quad 2-3 \quad 3-4 \quad 4-5 \quad 5-6 \quad 13-14 \quad 13-17 \quad 14-15 \quad 15-16 \quad 16-17$

Match level :

1:Atom 2:Atom 3:Atom 4:Atom 5:Atom 6:Atom 7:Atom 8:Atom 9:Atom 10:CLASS 11:CLASS 12:CLASS 13:Atom 14:Atom 15:Atom 16:Atom 17:Atom

L3 STRUCTURE UPLOADED

=> s 13 sss full

FULL SEARCH INITIATED 11:20:06 FILE 'REGISTRY' FULL SCREEN SEARCH COMPLETED - 3016 TO ITERATE

100.0% PROCESSED 3016 ITERATIONS

SEARCH TIME: 00.00.01

L40 SEA SSS FUL L3

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0 ANSWERS

```
1 2 3 4 5 6 7 8 9 13 14 15 16 17
ring/chain nodes :
10 11 12
ring/chain bonds :
7-11 8-12 9-10 12-13
ring bonds :
1-2 1-6 2-3 3-4 4-5 4-7 5-6 5-9 7-8 8-9 13-14 13-17 14-15 15-16 16-17
exact/norm bonds :
13-17 14-15
exact bonds :
4-7 5-9 7-8 7-11 8-9 8-12 9-10 12-13
normalized bonds :
1-2 1-6 2-3 3-4 4-5 5-6 13-14 15-16 16-17
```

Match level :

ring nodes :

1:Atom 2:Atom 3:Atom 4:Atom 5:Atom 6:Atom 7:Atom 8:Atom 9:Atom 10:CLASS 11:CLASS 12:CLASS 13:Atom 14:Atom 15:Atom 16:Atom 17:Atom

L5 STRUCTURE UPLOADED

=> s 15 sss full FULL SEARCH INITIATED 11:23:50 FILE 'REGISTRY' FULL SCREEN SEARCH COMPLETED - 5922 TO ITERATE

100.0% PROCESSED 5922 ITERATIONS 0 ANSWERS

SEARCH TIME: 00.00.01

ring nodes :

L6 0 SEA SSS FUL L5

Uploading C:\Documents and Settings\mpepitone\My Documents\ChemDraw\10572677\22.str

1 2 3 4 5 6 7 8 9 13 14 15 16 17 ring/chain nodes : 10 11 12 ring/chain bonds : 7-11 8-12 9-10 12-13 ring bonds : 1-2 1-6 2-3 3-4 4-5 4-7 5-6 5-9 7-8 8-9 13-14 13-17 14-15 15-16 16-17 exact/norm bonds : 13-17 14-15 exact bonds : 4-7 5-9 7-8 7-11 8-9 8-12 9-10 12-13 normalized bonds :

Match level : 1:Atom 2:Atom 3:Atom 4:Atom 5:Atom 6:Atom 7:Atom 8:Atom 9:Atom 10:CLASS 11:CLASS 12:CLASS 13:Atom 14:Atom 15:Atom 16:Atom 17:Atom

1-2 1-6 2-3 3-4 4-5 5-6 13-14 15-16 16-17

 ${\tt Uploading C:\locuments and Settings\mpepitone\My Documents\ChemDraw\10572677\8.str}$

```
ring nodes:
1 2 3 4 5 6 7 8 9
ring/chain nodes:
10 11 12 13 14 15 16 17 18 19
ring/chain bonds:
7-11 8-12 9-10 12-13 13-14 13-15 13-16 14-17 15-18 16-19
ring bonds:
1-2 1-6 2-3 3-4 4-5 4-7 5-6 5-9 7-8 8-9
exact/norm bonds:
12-13 13-14 13-15 13-16 14-17 15-18 16-19
exact bonds:
4-7 5-9 7-8 7-11 8-9 8-12 9-10
normalized bonds:
1-2 1-6 2-3 3-4 4-5 5-6
```

Match level :

1:Atom 2:Atom 3:Atom 4:Atom 5:Atom 6:Atom 7:Atom 8:Atom 9:Atom 10:CLASS 11:CLASS 12:CLASS 13:CLASS 14:CLASS 15:CLASS 16:CLASS 17:CLASS 18:CLASS 19:CLASS

L10 STRUCTURE UPLOADED

=> s 110 sss full STRUCTURE TOO LARGE - SEARCH ENDED A structure in your query is too large. You may delete attributes or atoms to reduce the size of the structure and try again.

_<

Uploading C:\Documents and Settings\mpepitone\My Documents\ChemDraw\10572677\6.str



chain nodes : 15 16 17 ring nodes : 1 2 3 4 5 6 7 8 9 ring/chain nodes : 10 11 12 13 chain bonds : 13-15 13-16 13-17 ring/chain bonds : 7-11 8-12 9-10 12-13 ring bonds : 1-2 1-6 2-3 3-4 4-5 4-7 5-6 5-9 7-8 8-9 exact/norm bonds : 12-13 13-15 13-16 13-17 exact bonds : 4-7 5-9 7-8 7-11 8-9 8-12 9-10 normalized bonds : 1-2 1-6 2-3 3-4 4-5 5-6

Match level: 1:Atom 2:Atom 3:Atom 4:Atom 5:Atom 6:Atom 7:Atom 8:Atom 9:Atom 10:CLASS 11:CLASS 12:CLASS 13:CLASS 15:CLASS 16:CLASS 17:CLASS

L12 STRUCTURE UPLOADED

=> s 112 sss full FULL SEARCH INITIATED 11:35:05 FILE 'REGISTRY' FULL SCREEN SEARCH COMPLETED - 2709 TO ITERATE

100.0% PROCESSED 2709 ITERATIONS 27 ANSWERS SEARCH TIME: 00.00.01

L13 27 SEA SSS FUL L12

=> file caplus
COST IN U.S. DOLLARS
SINCE FILE TOTAL
ENTRY SESSION
FULL ESTIMATED COST 189.24 986.54

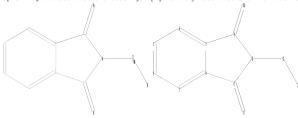
DISCOUNT AMOUNTS (FOR QUALIFYING ACCOUNTS) SINCE FILE TOTAL

REGISTRY includes numerically searchable data for experimental and predicted properties as well as tags indicating availability of experimental property data in the original document. For information on property searching in REGISTRY, refer to:

http://www.cas.org/support/stngen/stndoc/properties.html

= 3

Uploading C:\Documents and Settings\mpepitone\My Documents\ChemDraw\10572677\t.str



```
chain nodes:
13
ring nodes:
1 2 3 4 5 6 7 8 9
ring/chain nodes:
10 11 12
ring/chain bonds:
7-11 8-12 9-10 12-13
ring bonds:
1-2 1-6 2-3 3-4 4-5 4-7 5-6 5-9 7-8 8-9
exact bonds:
1-2 1-6 2-3 3-4 4-5 5-6
```

Match level: 1:Atom 3:Atom 4:Atom 5:Atom 6:Atom 7:Atom 8:Atom 9:Atom 10:CLASS 11:CLASS 12:CLASS 13:Atom

L15 STRUCTURE UPLOADED

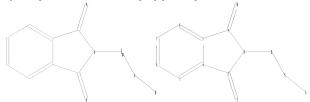
=> s 115 sss full FULL SEARCH INITIATED 11:39:24 FILE 'REGISTRY' FULL SCREEN SEARCH COMPLETED - 268242 TO ITERATE

100.0% PROCESSED 268242 ITERATIONS SEARCH TIME: 00.00.05

60140 ANSWERS

L16 60140 SEA SSS FUL L15

Uploading C:\Documents and Settings\mpepitone\My Documents\ChemDraw\10572677\nhy.str



chain nodes : 13 16 ring nodes : 1 2 3 4 5 6 7 8 9 ring/chain nodes : 10 11 12 chain bonds : 13 - 16ring/chain bonds : 7-11 8-12 9-10 12-13 ring bonds : 1-2 1-6 2-3 3-4 4-5 4-7 5-6 5-9 7-8 8-9 exact/norm bonds : 13-16 exact bonds : 4-7 5-9 7-8 7-11 8-9 8-12 9-10 12-13 normalized bonds : 1-2 1-6 2-3 3-4 4-5 5-6

Match level: 1:Atom 3:Atom 4:Atom 5:Atom 6:Atom 7:Atom 8:Atom 9:Atom 10:CLASS 11:CLASS 12:CLASS 13:Atom 16:Atom

L17 STRUCTURE UPLOADED

=> s 117 sss full FULL SEARCH INITIATED 11:41:44 FILE 'REGISTRY' FULL SCREEN SEARCH COMPLETED - 266737 TO ITERATE

100.0% PROCESSED 266737 ITERATIONS 2397 ANSWERS SEARCH TIME: 00.00.08

L18 2397 SEA SSS FUL L17

=> file caplus
COST IN U.S. DOLLARS
SINCE FILE TOTAL
ENTRY SESSION
FULL ESTIMATED COST 373.20 1436.06

DISCOUNT AMOUNTS (FOR QUALIFYING ACCOUNTS) SINCE FILE TOTAL

DISCOUNT AMOUNTS (FOR QUALIFYING ACCOUNTS)

SINCE FILE TOTAL ENTRY SESSION 0.00 -17.22

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STRUCTURE FILE UPDATES: 19 AUG 2009 HIGHEST RN 1174705-31-7 DICTIONARY FILE UPDATES: 19 AUG 2009 HIGHEST RN 1174705-31-7

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http://www.cas.org/support/stngen/stndoc/properties.html

=>

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chain nodes:
13 14
ring nodes:
1 2 3 4 5 6 7 8 9
ring/chain nodes:
10 11 12
chain bonds:
12-13 13-14
ring/chain bonds:
7-11 8-12 9-10
ring bonds:
12-1 3-12 9-10

=> STR 671180-46-4

WARNING. SINGLE ATOM FRAGMENTS NOT INCLUDED IN MODEL: Br

: END

L29 STRUCTURE CREATED

=> S L29 FAM FUL

FULL SEARCH INITIATED 11:52:43 FILE 'REGISTRY'
FULL SCREEN SEARCH COMPLETED - 27 TO ITERATE

100.0% PROCESSED 27 ITERATIONS

SEARCH TIME: 00.00.01

L30 2 SEA FAM FUL L29

=>

=> D SCAN

L30 2 ANSWERS REGISTRY COPYRIGHT 2009 ACS on STN

IN 1H-Isoindole-1,3(2H)-dione, 2-[10-(1H-imidazol-1-yl)decyl]-

MF C21 H27 N3 O2

CI COM

PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

HOW MANY MORE ANSWERS DO YOU WISH TO SCAN? (1):1

L30 2 ANSWERS REGISTRY COPYRIGHT 2009 ACS on STN

IN 1H-Isoindole-1,3(2H)-dione, 2-[10-(1H-imidazol-1-yl)decyl]-, hydrobromide (1:1)

2 ANSWERS

(T:T)

MF C21 H27 N3 O2 . Br H